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September 21, 2004

Marianne Lamont Horinko, Administrator
U.S. Environmental Protection Agency
P.O. Box 1473
Merrifield, VA 2216

Attn: Chemical Right-to-Know Program

Re: EPA comments on the Test Plan and Robust Data Summary for Carbamic Acid[(Dimethylamino)iminomethyl]methyl-, ethyl ester, monohydrochloride.

Dear Administrator Horinko,

E. I. du Pont de Nemours & Company, Inc. received EPA's comments on the test plan and robust data summary for carbamic acid[(dimethylamino)iminomethyl]methyl-, ethyl ester, monohydrochloride and is pleased to respond. We have considered the recommended revisions to the substance characterization, physiochemical properties, environmental fate, health effects, and ecological effects. We have revised our submittal as needed on the attached summary sheet. Also included with this submittal is a revised robust data summary.

Please feel free to contact me with any questions or concerns you may have with regards to this submission at Edwin.L.Mongan-1@usa.dupont.com or by phone at 302-773-0910.

Sincerely,

Edwin L. Mongan, III
Manager, Environmental Stewardship
DuPont Safety, Health & Environment

Cc: Charles Auer – U.S. EPA
Office of Pollution Prevention & Toxics
U. S. Environmental Protection Agency
401 M Street, SW
Washington, DC 20460

September 21, 2004

Carbamic acid[(dimethylamino)iminomethyl]methyl-, ethyl ester, monohydrochloride:
Response to EPA Comments

Substance Characterization

EPA Comment: The submitter needs to clarify whether a solid product occurs in the manufacturing process.

Response: There is no solid product in the process.

Physiochemical Properties

EPA Comment: *Melting point, boiling point, vapor pressure, water solubility.* Adequate data are available for these endpoints for the purposes of the HPV Challenge Program, if a preformulation non-aqueous product is not isolate. Otherwise, measured data need to be generated according to OECD guideline.

Response: A preformulation, non-aqueous product is not isolated in this process.

EPA Comment: *Partition coefficient.* The submitter reported a log Kow of -0.07 using KOWWIN v.1.66. EPA obtained this value using a SMILES notation of CCOC(=O)N(C)C=NN(C)C. This notation does not represent the structure of carbamate hydrochloride. The correct notation is O=C(OCC)N(C)C(+N(H)(H)(Cl))N(C)C, which produces a value of -3.96. The submitter needs to use the correct SMILES notation and recalculate the partition coefficient.

Response: The partition coefficient was recalculated using the correct SMILES notation. The ECOSAR models for aquatic toxicity endpoints were also rerun using the correct SMILES notation.

Environmental Fate

EPA Comment: *Photodegradation.* The submitter needs to provide data for this endpoint, estimated data using EPIWIN are acceptable.

Response: EPIWIN data were added to the document.

EPA Comment: *Stability in water.* The test plan reports that this chemical hydrolyzes very slowly (>10 years at pH 7, estimate from HYDROWIN V. 1.67). The submitter needs to provide measured data.

Response: A stability in water test was added to the test plan.

EPA Comment: *Biodegradation.* The submitter indicated that carbamate hydrochloride is readily biodegradable as estimated using BIOWIN. This conclusion cannot be inferred from estimated data. The submitter needs to provide measured biodegradation data following OECD TG 301.

September 21, 2004

Response: A biodegradation test following OECD TG 301 was added to the test plan.

EPA Comment: *Fugacity*. The submitter's use of Level III model is adequate. However, the submitter needs to recalculate its fugacity model using appropriately corrected or measured physiochemical values. The submitter also needs to include the input values used for the fugacity estimation.

Response: The fugacity model will be rerun once stability in water tests are completed. Current input values were added to the document.

Health Effects

EPA Comment: *Closed system intermediate status*. The submitter needs to provide additional information to satisfy the requirements for classification of carbamate hydrochloride as a 'closed system intermediate.' Or as an alternative to the developmental test proposed, per HPV Challenge Program guidance, EPA recommends a combined repeated dose/reproductive/developmental screening test (OECD 421 or 422).

Response: While DuPont uses carbamate hydrochloride as a closed system intermediate, we will conduct the combined repeated dose/reproductive/developmental-screening test (OECD 422) to meet the requirements of the developmental toxicity, repeated dose, and the reproductive toxicity endpoints.

Ecological Effects

EPA comment: The submitter needs to supply the missing log Kow input value used to obtain the predicted values from the ECOSAR model so that an independent evaluation can be made.

Response: Corrected log Kow input values were added to the document.

**OVERALL SUMMARY FOR CARBAMIC
ACID[(DIMETHYLAMINO)IMINOMETHYL]METHYL-, ETHYL ESTER,
MONOHYDROCHLORIDE**

Summary

Carbamic Acid[(Dimethylamino)iminomethyl]methyl-, ethyl ester, monohydrochloride is a solid that is soluble in water at greater than 50% concentration. This chemical is also referred to in this document as carbamate hydrochloride or F3455.HCl. No data are available on its melting point, and boiling point, density, and vapor pressure data are not applicable to this chemical. The product as shipped is a liquid, which contains F3455.HCl (35-51%), water (34-40%), dimethylamine hydrochloride (5-14%), and trimethylguanidine hydrochloride (1-5%). The product as shipped has a boiling point of 105°C, a liquid density of 69.7 lb/ft³ at 23°C, and a vapor pressure of 18 mm Hg at 21°C.

Environmental fate data for F-3455.HCl are generally not available. A review of estimated physical-chemical properties and environmental-fate characteristics based on output from EPIWIN 3.05 modeling software (Syracuse Research Corporation) indicates that F-3455.HCl is unlikely to represent a hazard as a persistent and/or bioaccumulative chemical (See Table 1). When modeled using a Level III fugacity model under a standard scenario of equal emissions to air, water, and soil, F-3455.HCl is expected to partition primarily into soil and water compartments. When dissolved in water at environmental pH, F-3455.HCl is expected to be mostly in an ionized form. Hydrolytic decomposition is not expected to readily transform F-3455.HCl, but F-3455.HCl may be subject to aqueous photolysis. In an indirect photolysis model (AOPWIN), the estimated half-life due to vapor phase OH radical reaction is 5.01 hours. Based on the BIOWIN ultimate survey model, F-3455.HCl, is expected to readily biodegrade. Because some inconsistencies were recognized in the modeling results for biodegradation, a ready biodegradability test, OECD 301, will be run. Hydrolysis testing, OECD 111, will also be run in order to address uncertainties about stability in water.

Table 1 : Environmental Fate

Bioaccumulation*	BCF = 3.162
Biodegradation*	Readily biodegradable
Fugacity*	Level III Partition Estimate Air 0.005 % Water 45 % Soil 54.9 % Sediments 0.08 %
* Modeled data	

No aquatic toxicity information was available on carbamate hydrochloride. Modeling of physical-chemical parameters (i.e., log Kow) and aquatic toxicity was conducted to help provide insight into the behavior in the environment and the aquatic toxicity of F3455.HCl (See Table 2). Syracuse Research Corporation models for estimating physical-chemical properties were used to estimate log₁₀ Kow (Meylan and Howard, 1995) for subsequent use in the ECOSAR program. ECOSAR (Meylan and Howard, 1999) was used to estimate aquatic toxicity data for green algae, daphnids (planktonic freshwater crustaceans), and fish. ECOSAR predictions are based on actual toxicity test data for classes of compounds with similar modes of action. The ECOSAR predictions indicate that F3455.HCl is unlikely to be acutely toxic to algae, invertebrates, or fish at environmentally relevant concentrations. Since there are no analog chemicals with existing test data to lend support to the modeled data, acute toxicity screening tests are proposed with fish, *Daphnia*, and algae.

Table 2: Predicted Aquatic Toxicity Values

Parameter	Estimated Value
Log Kow	-3.96 @ 25°C
96-hour LC ₅₀ (fish)	6.22x10 ⁷ mg/L
48-hour EC ₅₀ (daphnid)	4.42x10 ⁷ mg/L
96-hour EC ₅₀ (green algae)	1.96x10 ⁷ mg/L

The product as shipped has very low acute oral toxicity with an acute lethal dose (ALD) > 11,000 mg/kg in rats. Lethargy was observed on the day of dosing in animals administered 7500 and 11,000 mg/kg. Slight initial weight loss was evident at 670, 1500, 3400, 7500, and 11,000 mg/kg.

No data regarding genetic toxicity was found. Therefore, an *in vitro* bacterial reverse mutation assay and *in vitro* clastogenicity study in human peripheral blood lymphocytes following OECD guidelines 471 and 473, respectively are proposed.

No data regarding developmental, repeated dose toxicity or reproductive toxicity was found; therefore, a combined repeated dose/reproductive/developmental toxicity screening test (OECD 422) will be conducted. DuPont handles carbamate hydrochloride as an isolated intermediate.¹ While classification as such would alleviate the need to conduct a repeated dose and reproductive toxicity study, a developmental toxicity study would still be needed to satisfy the program requirements. Since the OECD 422 study would satisfy the developmental toxicity endpoint as well as provide repeated dose and reproductive data, this test was selected.

¹ As defined by EPA guidance, an isolated intermediate is one in which there is controlled transport, i.e. to a limited number of locations within the same company or second parties that use the chemical in a controlled way as an intermediate with a well known technology.

September 21, 2004

Human Exposure Information

F3455.HCl is manufactured at the DuPont Belle Plant and shipped to the DuPont LaPorte Plant. DuPont LaPorte is the only customer. The sites can have from 2 to 10 personnel working (construction, contractor, and plant employees) in the F3455.HCl operating areas. The areas where the substance is manufactured will have 2 operators present per shift during normal operations and 5 to 10 people during a shutdown or major construction activity.

The F3455.HCl is not present in the distributed product. There are a series of chemical reaction steps, and the F3455.HCl is consumed by chemical reaction. Chemical analysis of the product sold in commerce shows no detectable amount. The detection limit is estimated to be 0.1 wt% based on liquid chromatography.

Transport between the two locations is via dedicated rail cars or trucks. The F3455.HCl is shipped in bulk as the hydrochloride salt in water. Annual volume is 2.5-3 million pounds transported.

Controls during transport and transfer at the dispatching and receiving site are designed to ensure a closed system. This solution is pumped directly from the reactor to the railcar or truck for shipment. Normal shipment is by railcar. During loading of the railcar, the railcar dome is vented to the atmosphere. Because the aqueous salt solution has a low vapor pressure, the only significant exposure risk is as a result of a spill during loading of the railcar or truck. For railcars, spill containment including a stainless steel catch pan with a double-lined sump is provided for spill protection. Railcars are inspected to maintain the integrity of the fleet. The bottom valve of tank cars or trucks is checked by DuPont Belle operators when loading first starts (plug is removed to look for any liquid that may have leaked through the valve). The operator who loads the car wears appropriate PPE to guard against splashes. A checklist is completed for each shipment, to ensure that standard procedures are followed. Any spills, water used to wash equipment, etc., is sent to the biological treatment system on-site.

On receipt of the product at DuPont LaPorte, the solution is again handled in a closed system that includes pumping from the railcar or truck to the storage tank. It is consumed in the manufacturing process in a closed pipe and reactor system. The only significant exposure risk is during the unloading operation. The unloading spot is equipped with spill containment (catch pan) and the storage tank is diked. Any spills in these containment areas are disposed of by on-site incineration or biological treatment. Both the unloading spot and the storage tank vent to a flare. Unloading operators or others that might perform first breaks into equipment wear PPE to guard against splashes.

DuPont handles carbamate hydrochloride as an isolated intermediate.² While classification as such would alleviate the need to conduct a repeated dose and reproductive toxicity study, a developmental toxicity study would still be needed to satisfy the program requirements. Since

² As defined by EPA guidance, an isolated intermediate is one in which there is controlled transport, i.e. to a limited number of locations within the same company or second parties that use the chemical in a controlled way as an intermediate with a well known technology.

September 21, 2004

the OECD 422 study would satisfy the developmental toxicity endpoint as well as provide some repeated dose and reproductive data, this test will be conducted.

References for the Summary

Meylan, W. M. and P. H. Howard (1995). J. Pharm. Sci., 84:83-92.

Meylan, W. M. and P. H. Howard (1999). User's Guide for the ECOSAR Class Program, Version 0.993 (Mar 99), prepared for J. Vincent Nabholz and Gordon Cas, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington, DC, prepared by Syracuse Research Corp., Environmental Science Center, Syracuse, NY 13210 (submitted for publication).

September 21, 2004

**TEST PLAN FOR CARBAMIC
ACID[(DIMETHYLAMINO)IMINOMETHYL]METHYL-, ETHYL ESTER,
MONOHYDROCHLORIDE**

Carbamate Hydrochloride CAS No. 65086-85-3	Data Available	Data Acceptable	Testing Required
Study	Y/N	Y/N	Y/N
PHYSICAL/CHEMICAL CHARACTERISTICS			
Melting Point	Y	Y	N
Boiling Point	Y	Y	N
Vapor Pressure	Y	Y	N
Partition Coefficient	Y	Y	N
Water Solubility	Y	Y	N
ENVIRONMENTAL FATE			
Photodegradation	Y	Y	N
Stability in Water	Y	N	Y
Transport (Fugacity)	Y	Y	N
Biodegradation	Y	N	Y
ECOTOXICITY			
Acute Toxicity to Fish	Y	N	Y
Acute Toxicity to Invertebrates	Y	N	Y
Acute Toxicity to Aquatic Plants	Y	N	Y
MAMMALIAN TOXICITY			
Acute Toxicity	Y	Y	N
Repeated Dose Toxicity	N	N	Y
Developmental Toxicity	N	N	N
Reproductive Toxicity	N	N	N
Genetic Toxicity Gene Mutations	N	N	Y
Genetic Toxicity Chromosomal Aberrations	N	N	Y
Y = Yes N= No N/A = Not Applicable			

**ROBUST SUMMARY FOR CARBAMIC
ACID[(DIMETHYLAMINO)IMINOMETHYL]METHYL-, ETHYL ESTER,
MONOHYDROCHLORIDE**

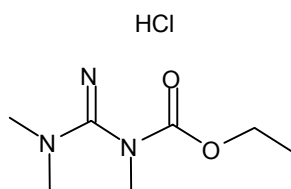
Existing published and unpublished data were collected and scientifically evaluated to determine the best possible study or studies to be summarized for each required endpoint. In the spirit of this voluntary program, other data of equal or lesser quality are not summarized, but are listed as related references at the end of each appropriate section, with a statement to reflect the reason why these studies were not summarized.

1.0 Substance Information

CAS Number: 65086-85-3

Chemical Name: Carbamic acid[(dimethylamino)iminomethyl]methyl-, ethyl ester, monohydrochloride

Structural Formula:



Other Names: Carbamate hydrochloride

Carbamic acid, (aminoiminomethyl)methyl-, dimethyl deriv., ethyl ester monohydrochloride

F-3455.HCl

Exposure Limits: No Data.

2.0 Physical – Chemical Properties

2.1 Melting/Freezing Point:

Value:	F3455.HCl: No Data Product as shipped: -49.4°C (Freezing Point)
Decomposition:	No Data
Pressure:	No Data
Method:	No Data
GLP:	Unknown
Reference:	DuPont Co. (1996). Material Data Safety Sheet No. B0000006 (May 24).
Reliability:	Not assignable because limited study information was

available.

Additional References for Boiling Point: None Found.

2.2 Boiling Point:

Value:	F3455.HCl: Not applicable Product as shipped: 105°C
Decomposition:	No Data
Pressure:	No Data
Method:	No Data
GLP:	Unknown
Reference:	DuPont Co. (1996). Material Data Safety Sheet No. B0000006 (May 24).
Reliability:	Not assignable because limited study information was available.

Additional References for Boiling Point: None Found.

2.3 Density:

Value:	F3455.HCl: Not applicable Product as shipped: 69.7 lb/ft ³
Temperature:	23°C
Method:	No Data
GLP:	Unknown
Results:	No additional data.
Reference:	DuPont Co. (1996). Material Data Safety Sheet No. B0000006 (May 24).
Reliability:	Not assignable because limited study information was available.

Additional References for Density: None Found.

2.4 Vapor Pressure:

Value:	F3455.HCl: Not applicable Product as shipped: 18 mm Hg
Temperature:	21°C
Decomposition:	No Data
Method:	No Data
GLP:	Unknown
Reference:	DuPont Co. (1996). Material Data Safety Sheet No. B0000006 (May 24).
Reliability:	Not assignable because limited study information was available.

Additional References for Vapor Pressure: None Found.

2.5 Partition Coefficient (log Kow):

Value: F-3455.HCl: -3.96
Temperature: 25°C
Method: Modeled. KOWWIN, v. 1.66, module of EPIWIN 3.05 (Syracuse Research Corporation).

KOWWIN uses “fragment constant” methodologies to predict log P.
GLP: Not applicable
Reference: Meylan, W. M. and P. H. Howard (1995). J. Pharm. Sci., 84:83-92.
Reliability: Estimated based on an accepted model.

Additional References for Partition Coefficient (log Kow): None Found.

2.6 Water Solubility:

Value: F3455.HCl: At least 50%
Product as shipped: Infinite
Temperature: No Data
pH/pKa: No Data
Method: No Data
GLP: Unknown
Reference: DuPont Co. (2000). Unpublished Data.
Reliability: Not assignable because limited study information was available.

Additional References for Water Solubility: None Found.

2.7 Flash Point:

Value: F3455.HCl: Not applicable
Product as shipped: 60°C
Method: TCC
GLP: Unknown
Reference: DuPont Co. (1996). Material Data Safety Sheet No. B0000006 (May 24).
Reliability: Not assignable because limited study information was available.

Additional References for Flash Point: None Found.

2.8 Flammability: No Data.

3.0 Environmental Fate

3.1 Photodegradation:

Concentration:	No Data
Temperature:	No Data
Direct Photolysis:	Inspection of F-3455.HCl indicates that it may be subject to aquatic photodegradation.
Indirect Photolysis:	The estimated half-life due to vapor phase OH radical reaction is 5.01 h.
Breakdown Products:	No Data
Method:	Inspection of chemical structure
GLP:	Not Applicable
Reference:	Direct Photolysis: Harris, J. C. (1990). Rate of Aqueous Photolysis, Chapter 8 In Lyman, W. J. et al. (eds.). <u>Handbook of Chemical Property Estimation Methods</u> , American Chemical Society, Washington, DC.
	Indirect Photolysis: AOPWIN, v. 1.91 module of EPIWIN 3.11. Meylan, W. M. and P. H. Howard (1993). <u>Chemosphere</u> , 26:2293-99.
Reliability:	Estimate based on known qualitative structure-activity relationships.

Additional References for Photodegradation: None Found.

3.2 Stability in Water:

Concentration:	No Data
Half-life:	Hydrolyses very slowly (> 10 years at pH 7) in water.
% Hydrolyzed:	No Data
Method:	Modeled. HYDROWIN, v. 1.67 module of EPIWINN v3.05 (Syracuse Research Corporation). HYDROWIN estimates aqueous hydrolysis rate constants for the following chemical classes: esters, carbamates, epoxides, halomethanes and selected alkyl halides. HYDROWIN estimates acid- and base-catalyzed rate constants; it does NOT estimate neutral hydrolysis rate constants. The prediction methodology was developed for the U.S. Environmental Protection Agency and is outlined in Mill et al., 1987.
GLP:	Not Applicable
Reference:	Mill, T. et al. (1987). "Environmental Fate and Exposure Studies Development of a PC-SAR for Hydrolysis: Esters,

Alkyl Halides and Epoxides” EPA Contract No. 68-02-4254,
SRI International Menlo Park, CA.

Reliability: Estimate based on an accepted model.

Additional References for Stability in Water: None Found.

3.3 Transport (Fugacity):

Media: For F-3455.HCl
Air, Water, Soil, and Sediments

Compartment	% of total distribution	½ life (hours) (advection + reaction)
Air	0.005	15.1
Water	45	360
Soil	54.9	720
Sediment	0.08	3240

SMILES: O=C(OCC)N(C)C(=N(H)(H)(Cl))N(C)C

Molecular Weight: 209.68

Henry's Law Constant: $2.88\text{e-}019 \text{ atm-m}^3/\text{mole}$
(HENRYWIN program)

Vapor Pressure: $1.37\text{e-}007 \text{ mm Hg}$ (MPBPWIN program)

Liquid Vapor Pressure: $3.82\text{e-}006 \text{ mm Hg}$ (super-cooled)

Melting Point: 171°C (MPBPWIN program)

Log Kow: -3.96 (KOWWIN program)

Soil Koc: $4.5\text{e-}005$ (calc by model)

Log Koc = 0.349

Adsorption
Coefficient:

Desorption:

Volatility:

Method:

No Data

Henry's Law Constant = $1.53 \times 10^{-10} \text{ atm-m}^2/\text{mole}$

Modeled, using 50% (w/v) water solubility value.

Henry's Law Constant - HENRYWINN v. 3.10 module of EPIWINN v3.05 (Syracuse Research Corporation). Henry's Law Constant (HLC) is estimated by two separate methods that yield two separate estimates. The first method is the bond contribution method and the second is the group contribution method. The bond contribution method is able to estimate many more types of structures; however, the group method estimate is usually preferred (but not always) when all fragment values are available.

Log Koc – Calculated from log Kow by the Mackay Level III fugacity model incorporated into EPIWINN v3.05 (Syracuse Research Corporation).

Environmental Distribution - Mackay Level III fugacity model, in EPIWINN v3.05 (Syracuse Research Corporation). Emissions (1000 kg/hr) to air, water, and soil compartments.

GLP: Not Applicable

Reference: HENRYWIN – Hine, J. and P. K. Mookerjee (1975). J. Org. Chem., 40(3):292-8 and Meylan, W. and P. H. Howard (1991). Environ. Toxicol. Chem., 10:1283-93.

Fugacity - The methodology and programming for the Level III fugacity model incorporated into EPIWIN v3.05 (Syracuse Research Corporation) were developed by Dr. Donald MacKay and coworkers and are detailed in: Mackay, D. (1991). Multimedia Environmental Models: The Fugacity Approach, pp. 67-183, Lewis Publishers, CRC Press.

Mackay, D. et al. (1996). Environ. Toxicol. Chem., 15(9):1618-1626.

Mackay, D. et al. (1996). Environ. Toxicol. Chem., 15(9):1627-1637.

Reliability: Estimated values based on accepted model.

Additional References for Transport (Fugacity): None Found.

3.4 Biodegradation:

Value: Estimated half-life: 15 days, estimated to be readily biodegradable

Ultimate Biodegradation Timeframe: Weeks

Breakdown Products: No Data

Method: Modeled. BIOWIN, v. 4.0 module of EPINWINN v3.05 (Syracuse Research Corporation). BIOWIN estimates the probability for the rapid aerobic biodegradation of an organic chemical in the presence of mixed populations of environmental microorganisms. Estimates are based upon fragment constants that were developed using multiple linear and non-linear regression analyses.

GLP: Not applicable

Reference: Boethling, R. S. et al. (1994). Environ. Sci. Technol., 28:459-65.

Howard, P. H. et al. (1992). Environ. Toxicol. Chem., 11:593-603.

Howard, P. H. et al. (1987). Environ. Toxicol. Chem., 6:1-

10.

Tunkel, J. et al. (2000). "Predicting Ready Biodegradability in the MITI Test" Environ. Toxicol. Chem., accepted for publication.

Reliability: Estimated value based on accepted model.

Additional References for Biodegradation: None Found.

3.5 Bioconcentration:

Value: BCF = 3.162

Method: Modeled. BCFWIN v. 2.4 module of EPINWINN v3.05 (Syracuse Research Corporation). BCFWIN estimates the bioconcentration factor (BCF) of an organic compound using the compound's log octanol-water partition coefficient (Kow) with correction factors based on molecular fragments.

GLP: Not applicable

Reference: "Improved Method for Estimating Bioconcentration Factor (BCF) from Octanol-Water Partition Coefficient", SRC TR-97-006 (2nd Update), July 22, 1997; prepared for: Robert S. Boethling, EPA-OPPT, Washington, DC; Contract No. 68-D5-0012; prepared by: William M. Meylan, Philip H. Howard, Dallas Aronson, Heather Printup and Sybil Gouchie; Syracuse Research Corp.

Reliability: Estimated value based on accepted model.

Additional References for Bioconcentration: None Found.

4.0 Ecotoxicity

4.1 Acute Toxicity to Fish:

Type: 96-hour LC₅₀

Species: Fish

Value: 6.22x10⁷ mg/L(log₁₀ Kow of -3.96)

Method: Modeled

GLP: Not Applicable

Test Substance: F3455.HCl

Results: No additional data.

Reference: Meylan, W. M. and P. H. Howard (1999). User's Guide for the ECOSAR Class Program, Version 0.993 (Mar 99), prepared for J. Vincent Nabholz and Gordon Cas, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington, DC, prepared by Syracuse Research Corp., Environmental Science Center, Syracuse, NY 13210 (submitted for publication).

Reliability: Estimated value based on accepted model.

Additional References for Acute Toxicity to Fish: None Found.

4.2 Acute Toxicity to Invertebrates:

Type: 48-hour EC₅₀
Species: Daphnid
Value: 4.42x10⁷ mg/L(log₁₀ Kow of -3.96)
Method: Modeled
GLP: Not Applicable
Test Substance: F3455.HCl
Results: No additional data.
Reference: Meylan, W. M. and P. H. Howard (1999). User's Guide for the ECOSAR Class Program, Version 0.993 (Mar 99), prepared for J. Vincent Nabholz and Gordon Cas, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington, DC, prepared by Syracuse Research Corp., Environmental Science Center, Syracuse, NY 13210 (submitted for publication).
Reliability: Estimated value based on accepted model.

Additional References for Acute Toxicity to Invertebrates: None Found.

4.3 Acute Toxicity to Aquatic Plants:

Type: 96-hour EC₅₀
Species: Green algae
Value: 1.96x10⁷ mg/L (log₁₀ Kow of -3.96)
Method: Modeled
GLP: Not Applicable
Test Substance: F3455.HCl
Results: No additional data.
Reference: Meylan, W. M. and P. H. Howard (1999). User's Guide for the ECOSAR Class Program, Version 0.993 (Mar 99), prepared for J. Vincent Nabholz and Gordon Cas, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington, DC, prepared by Syracuse Research Corp., Environmental Science Center, Syracuse, NY 13210 (submitted for publication).
Reliability: Estimated value based on accepted model.

Additional References for Acute Toxicity to Aquatic Plants: None Found.

5.0 Mammalian Toxicity

5.1 Acute Toxicity:

Type:	Oral ALD
Species/Strain:	Rats/ChR-CD
Value:	> 11,000 mg/kg
Method:	No specific test guideline was reported; however, a scientifically defensible approach was used to conduct the study.
	The test material, in original form, or as a solution in water, was administered to young adult male rats in single doses via intragastric intubation. Dose levels of 670, 1000, 1500, 2250, 3400, 5000, 7500, and 11,000 mg/kg were tested. One male rat was tested at each dose level. Survivors were sacrificed 13 or 14 days after dosing without pathological examinations.
GLP:	No
Test Substance:	Product as shipped (which contains 42% F3455.HCl)
Results:	No mortality was observed. Lethargy was observed on the day of dosing at 7500 and 11,000 mg/kg. Slight initial weight loss was evident at 670, 1500, 3400, 7500, and 11,000 mg/kg.
Reference:	DuPont Co. (1974). Unpublished Data, Haskell Laboratory Report No. 70-74 "Acute Oral Test" (February 13).
Reliability:	High because a scientifically defensible or guideline method was used.

Additional References for Acute Oral Toxicity: None Found.

Type:	Inhalation Toxicity: No Data.
Type:	Dermal Toxicity: No Data
Type:	Dermal Irritation: No Data.
Type:	Dermal Sensitization: No Data.
Type:	Eye Irritation: No Data.

September 21, 2004

5.2 Repeated Dose Toxicity: No Data.

5.3 Developmental Toxicity: No Data.

5.4 Reproductive Toxicity: No Data.

5.5 Genetic Toxicity:

Type: *In vitro* Genetic Toxicity Studies: No Data.

Type: *In vivo* Genetic Toxicity Studies: No Data.